Investigations of complex objects through coherent x-ray diffraction in the Bragg geometry

Ross Harder*[1]*, Meng Liange[2], Ian Robinson[1]

[1]London Centre for Nanotechnology, UK , [2]University of Illinois Urbana-Champaign

Our group, operating the coherent X-ray Diffraction (CXD) Beamline 34-ID-C at APS, has systematically studied the structure of nanocrystals by inversion of three dimensional coherent diffraction measured in the Bragg geometry. For various interesting reasons, including lattice distortions within the crystal, the measured diffraction is often not symmetric about the Bragg spot. This in turn leads to the recovery of complex density functions upon successful Fourier inversion.

We have frequently found that this phasing/inversion step fails to converge to acceptable error metrics, while at the same time producing acceptable looking images of smoothly connected electron density. Careful inspection of the resulting images found them to contain phase vortices, previously known to cause 'stagnation' in the convergence of iterative algorithms. In this case however the vortices occur in direct space outside of the support region defining the complex object. We have therefore introduced an adaptation of the Error Reduction(ER) algorithm. This form of ER removes the phase vortices in direct space while not destroying the recovered object, as traditional Error Reduction seemed to do. The details of these technique developments, illustrated with inversions of diffraction from a variety of nanocrystal and nanowire samples, will be presented.